

1-Nitrobutane

627-05-4 | DTXSID8020967

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -46.4 °C

Global applicability domain: Inside

Local applicability domain index: 8.90e-01

Confidence level: 3.66e-01

Nearest Neighbors from the Training Set

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1-Nitrobutane

Measured: -81.3

Predicted: -46.4

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Propane, 2-methyl-1-nitro-

Measured: -76.9

Predicted: -40.3

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Propane, 2-methyl-2-nitro-

Measured: 26.2

Predicted: -20.5

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3-Methyl-1-nitrobutane

Measured: 97.0

Predicted: 31.6

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1-Nitropropane

Measured: -108

Predicted: -87.7